EXCHANGE INTERACTION BETWEEN ELECTRONS IN METALS CONTAINING IMPURITIES AT FINITE TEMPERATURES

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Submitted March 30, 1967

Zh. Eksp. Teor. Fiz. 53, 1038–1052 (September, 1967)

Scattering of electrons in metals by impurities possessing a spin is considered at finite temperatures. The problem is solved with the aid of the unitarity relations for the scattering amplitude and its analytic properties. An expression for the scattering amplitude, valid throughout the temperature range of interest, is obtained. A relation between the amplitude and the one-electron Green's function in the approximation of small impurity concentrations is also indicated. The problem of impurity conductivity is then considered. The expression for the conductivity significantly depends on the sign of the spin-dependent part of the interaction between the electrons and impurities. When this sign is positive the conductivity at T = 0 is a maximum and when it is negative the conductivity has a sharp minimum. The latter circumstance permits one to qualitatively explain the experimental data pertaining to the maximum of the resistance of a number of alloys containing impurities with spin. At high temperatures the expression for the conductivity is essentially the same as that previously derived by Kondo.[2]

$\mathbf{I}$N an earlier paper[1] (henceforth cited as I) we investigated the scattering at zero temperature of an electron in a metal by an impurity having a spin. In the present article we generalize the results obtained in I to the case $T \neq 0$. The obtained expressions for the scattering amplitudes are valid in the entire region of temperatures of interest. It is possible to calculate with their aid the impurity conductivity of the metal. At high temperatures, the expression for the conductivity coincides essentially with the result obtained by Kondo.[2] At low temperatures, the expression for the conductivity depends on the sign of the constant which determines the spin part of the interaction with the impurity. In the case when this constant is positive, a simple approximate formula is obtained for the conductivity, valid for all T, and coinciding with the expression for the conductivity obtained from Abrikosov's paper;[3] if $T = 0$, then the conductivity is maximal in this case. However, if the interaction constant is negative, it becomes possible to obtain approximate formulas only in the region of low and high temperatures, and at $T = 0$ the conductivity is minimal. In the intermediate region, numerical integration is necessary in order to calculate the conductivity.

We define, in analogy with the case when $T = 0$, the scattering amplitude in the following manner:

$$F_{\alpha'\alpha}^{M'M}(E, \mathbf{k}, \mathbf{k}') = \frac{i}{4\pi} \int_{-\infty}^{'} dt\, dx\, dy\, e^{-i\mathbf{k}'\mathbf{x}+i\mathbf{k}\mathbf{y}} e^{iEt}$$
$$\times \left\langle M' \left| T\left(\left(i\frac{\partial}{\partial t} - H_0\right)_x \psi_{\alpha'}(\mathbf{x}, t), \psi_{\alpha}^+(\mathbf{y}, 0)\right) \right| M \right\rangle \left(i\frac{\partial}{\partial t} - H_0\right) , (1)$$

where $\langle M' | \ldots | M \rangle = (M' | \mathrm{Tr} e^{\beta(F-H)} \ldots | M)$, H is the complete Hamiltonian of the system, and the operation of taking the trace pertains only to the electronic variable systems, and not to the impurity spin projections.

Unlike the definition in I, we have introduced one of the derivatives with respect to the time under the T-product sign; it is easy to verify that both definitions coincide on the energy shell ($E_k = E_{k'} = E$). However, as will be shown below, off this shell expression (1) is

correct. We confine ourselves henceforth, just as in I, to the case of a pointlike scatterer, and disregard accordingly the dependence of the scattering amplitude on the vectors $\mathbf{k}$ and $\mathbf{k}'$.[1)]

For $T = 0$ the expression for the scattering amplitude was obtained by starting from the matrix element of the S matrix $(M'\mathbf{k}'\alpha | S | M\mathbf{k}\alpha)$. With the aid of a similar procedure we can show that

$$(M'| S^+ (a_{k'\alpha'} S a_{k\alpha}^+ - a_{k\alpha}^+ S a_{k'\alpha'} + S a_{k\alpha}^+ a_{k'\alpha'}$$
$$- a_{k'\alpha'} a_{k\alpha}^+ S) | M) = 2\pi i \delta(E_k - E_{k'}) 4\pi V^{-1} F_{\alpha'\alpha}^{M'M}(E_k); \quad (2)$$

in the left side we have carried out here a Gibbs averaging with Hamiltonian H_0. We note in this connection that it is actually perfectly immaterial whether the averaging in formula (1) is with the aid of H or H_0; this follows directly from expression (2), by virtue of which the averaging is carried out at the instant of time $t = -\infty$, when, in accordance with the usual assumptions concerning the adiabatic switching off of the interaction, both Hamiltonians coincide.[2)]

We introduce besides F also the retarded and advanced scattering amplitudes F_R and F_A, which can be obtained from the definition (1) by replacing in it the T-product by the retarded anticommutator and by the advanced one with the minus sign respectively. For all three amplitudes there exist integral representations analogous to the ordinary Lehmann expansions for the Green's function (see Appendix I), and with this, just as for the Green's function,

$$F = F_R(1-n) + F_A n, \quad n = \left(\exp \frac{E - E_F}{T} + 1\right)^{-1} \quad (3)$$

It follows from these representations that

[1)]Formally it follows from the fact that the operator ψ satisfies the equation $(i\, \partial/\partial t - H_0)\psi = v\psi$, where $V(\mathbf{x}) \sim \delta(\mathbf{x})$.

[2)]This can be verified also formally, by going over in (1) to the interaction representation and then carrying out the calculations by perturbation theory with the Hamiltonian H with the aid of a technique similar to that of Konstantinov and Perel'[4].

$$F_R(E) = A(E + i\delta) + B(E + i\delta)S\sigma,$$

$$F_A(E) = A(E - i\delta) + B(E - i\delta)S\sigma, \tag{4}$$

where S is the spin of the impurity, σ are Pauli matrices, and A and B are analytic functions of the complex variable E with a cut along the real axis from zero to infinity, where

$$A(E - i\delta) = A^*(E + i\delta), \quad B(E - i\delta) = B^*(E + i\delta).$$

The function F_R is connected in simple fashion with the single-electron Green's function G_R. We shall now show that in the limit of low impurity concentration we have the equality

$$G_R^{-1}(p, E) = G_0^{-1}(p, E) + 4\pi n_0 A(E + i\delta), \tag{5}$$

where n_0 is the concentration and G_R is the usual retarded single-electron Green's function. Just as in I, we assume that $m = \frac{1}{2}$, and neglect the interaction of the electrons with one another.

Let us consider first the single-electron Green's function in the case of one center:

$$G_R(x, x') = -i\vartheta(t - t')\langle M' | \{\psi(x), \psi^+(x')\} | M\rangle.$$

For it, obviously, there exists the equation

$$\left(i\frac{\partial}{\partial t} - H_0\right)_x G_R(x, x')\left(-i\frac{\partial}{\partial t'} - H_0\right)_{x'} = \delta(x - x')\left(-i\frac{\partial}{\partial t'} - H_0\right)_{x'}$$

$$-i\vartheta(t - t')\left\langle M' \left| \left\{ \left(i\frac{\partial}{\partial t} - H_0\right)\psi(x), \psi^+(x')\right\} \right| M\right\rangle\left(-i\frac{\partial}{\partial t'} - H_0\right)_{x'} \tag{6}$$

from which we can easily obtain, with the aid of the definition of F_R, the expression

$$G_R(\mathbf{x}, \mathbf{x}', E) = G_{0R}(\mathbf{x} - \mathbf{x}', E) - 4\pi F_R(E)G_{0R}(\mathbf{x}, E)G_{0R}(\mathbf{x}', E), \tag{7}$$

which is valid, of course, only in the case of a pointlike center. It is essentially this equality which justifies the introduction of the amplitude F_R by the method described above. On going to the case of many centers in the approximation where the density of these centers is small, each center should be taken into account only once. A procedure which is perfectly analogous to that described in the book of Abrikosov, Gor'kov, and Dzyaloshinskiĭ,[5] leads after averaging over the projections of the impurity spins to the formula (5).

Suhl has shown[6] that when $T \neq 0$ there exist for the amplitudes A and B the following unitarity conditions:

$$\text{Im } A = k[|A|^2 + |B|^2 S(S + 1)],$$

$$\text{Im } B = k[AB^* + A^*B - |B|^2(1 - 2n(E))]. \tag{8}$$

Here, and also everywhere throughout, unless specially stipulated, we assume that $E = E + i\delta$. It should be noted that Suhl has made a number of unjustified assumptions in the derivation of these formulas. In Appendix I we present a derivation of (8) that differs from Suhl's derivation. At the same time, there exist simple considerations that justify formula (8).

In I, in calculating the imaginary part of the amplitude, we discarded the contribution from the multiparticle intermediate state, basing ourselves on the fact that such states correspond to a small phase volume. On the other hand, all the terms of the perturbation-theory series for the retarded scattering amplitude can be divided into two classes. The first includes those terms in the series which contain only the integrals

over the single-particle intermediate states, that is, which can be represented in the form

$$\int f_1(\mathbf{k}', \mathbf{k}_1)(E_{k_1} - E_{k'})^{-1}f_2(\mathbf{k}_1, \mathbf{k}_2)(E_{k_2} - E_{k'})^{-1}$$

$$\times f_3(\mathbf{k}_2, \mathbf{k}_3)(E_{k_3} - E_{k'})^{-1} \ldots d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3, \tag{9}$$

where the functions f_i do not contain integrals of multiparticle intermediate states,[3] for example integrals of the type

$$\int dq_1 dq_2 dq_3 Z(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)\vartheta(q_1 - k_F)\vartheta(q_2 - k_F)$$

$$\times \vartheta(k_F - q_3)(E_{q_1} + E_{q_2} - E_{q_3} - E)^{-1}, \tag{10}$$

which correspond to three-particle states. All the remaining terms of the perturbation-theory series belong to the second class. It is obvious that summation of the series terms of the first class should lead to a scattering amplitude which satisfies the single-particle unitarity condition. Conversely, by "solving" these equations by perturbation theory we reproduce only those terms of the series which pertain to the first class.[4]

We note that such a solution can be obtained only for the amplitudes F_R and F_A, but not for F, since it is necessary during the course of the solution to reconstruct the amplitude from its imaginary part with the aid of the dispersion integral, which is possible only for analytic functions.

Thus, an analysis of the unitarity condition at $T = 0$ makes it possible to formulate a prescription for selecting the principal terms of the perturbation-theory series, and its "solution" is essentially a method for their summation.

Perturbation theory was not applicable for $T = 0$, owing to the divergence of the integrals over the intermediate states near the Fermi surface, since the integrands contained the functions $\vartheta(E_F - E)$. It is obvious that at finite temperatures, in all such integrals the step functions $\vartheta(E_F - E)$ are replaced by $n(E)$. It is clear that the unitarity condition to which these terms contribute will differ from the unitarity condition at $T = 0$ in that $\vartheta(E - E_F)$ is replaced by $1 - 2n$, which indeed leads to (8). As to the perturbation-theory series containing multiparticle intermediate states, the unitarity condition for them will again give a small contribution, since the smallness of the phase volume is retained also when $T \neq 0$. To this end it is sufficient that the temperatures be small compared with the degeneracy temperature.[5] When $T \neq 0$ generally speaking, additional terms of the perturbation-theory series can arise, but since the contribution from them vanishes at

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[3] We note that in our case f_i are complicated functions of the energy.

[4] The method of such a "solution," and also the proof that the solution variant chosen in I for the problem can be obtained by summation of items of the perturbation theory series, will be published separately. We note also that this problem was solved in a recent paper by Suhl and Wong [7] by a method which is close to the method of the present paper. However, the solution obtained in [7] does not correspond to the Hamiltonian used in I and in the present article. This is clear already from the fact that the expression obtained by Suhl and Wong for A decreases as $E \to \infty$ like E^{-1}, and not like $E^{-1/2}$. Inasmuch as the authors have actually employed the assumption that the interaction is pointlike, it is not clear whether there exists in general a reasonable Hamiltonian to which the solution obtained by them corresponds.

[9] We shall find below the scattering amplitude satisfying the conditions (8) for E, particularly for E far from the Fermi surface, where

T = 0, allowance for them goes beyond the limits of accuracy.

We now proceed to determine the scattering amplitude, starting from the conditions (8) and the analytic properties of A and B. The calculations will be carried out here in full analogy with the corresponding calculations of I.

We introduce in lieu of A and B the new amplitudes

$$a_+ = A + SB, \qquad a_- = A - (S+1)B. \tag{11}$$

with the aid of (8) we obtain for them the equations

$$\operatorname{Im} a_\pm = k\left\{ |a_\pm|^2 \pm \frac{2(S + 1/2 \mp 1/2)}{(2S+1)^2} |a_+ - a_-|^2 n(E) \right\}. \tag{12}$$

We write $\alpha_\pm$ in the form

$$a_\pm = \frac{1}{2ik}(\eta_\pm e^{2i\delta_\pm} - 1). \tag{13}$$

By virtue of (12) we have

$$\eta_\pm^2 = 1 \pm 2\frac{(S + 1/2 \pm 1/2)}{(2S+1)^2}[\eta_+^2 + \eta_-^2 - 2\eta_+\eta_-\cos 2(\delta_+ - \delta_-)]n(E), \tag{14}$$

from which, in particular, it follows that

$$(S+1)\eta_+^2 + S\eta_-^2 = 2S + 1. \tag{15}$$

We introduce in lieu of $\alpha_\pm$ the complex scattering phases

$$\varphi_\pm = -\frac{k}{4\pi}\int_0^\infty \frac{dE' \ln \eta_\pm^2(E')}{k'(E' - E - i\delta)} = \varphi_\pm' - \frac{i}{2}\ln\eta_\pm,$$
$$\delta_\pm = \nu_\pm + \varphi_\pm'. \tag{16}$$

Here, obviously, the functions

$$a_\pm' = \frac{1}{2ik}[(2ika_\pm + 1)e^{-2i\varphi_\pm} - 1] = \frac{1}{2ik}(e^{2i\nu_\pm} - 1) \tag{17}$$

will be analytic and the entire complex E plane, with a cut along the real axis from zero to infinity, and for them the "elastic" unitarity condition

$$\operatorname{Im} a_\pm' = k|a_\pm'|^2 \tag{18}$$

holds. Therefore, on the basis of the same considerations as in I (see also the footnote [4]) we have

$$a_\pm' = a_\pm(1 - ika_\pm)^{-1}, \qquad \nu_\pm = \operatorname{arctg} ka_\pm. \tag{19}$$

It will be shown below that the quantities $a_\pm$ in these formulas should equal the corresponding quantities from I.

Just as in I, following Suhl,[8] we introduce the function

$$u = \frac{1 + 2ikA}{B} = \frac{2S + 1 + 2ik[(S+1)a_+ + Sa_-]}{a_+ - a_-}, \tag{20}$$

for which we get by virtue of (8) and (12)

$$u(E + i\delta) - u(E - i\delta) = 2ik[1 - 2n(E)]. \tag{21}$$

Therefore u(E) can be represented in the form

$$u(E) = P(E) - \frac{4k^2}{\pi}\int_0^\infty dk'\frac{n(k'^2)}{k'^2 - k^2 - i\delta} + ik = u_1(E) + ik[1 - 2n(E)], \tag{22}$$

where P(E) is a rational function.

From (20), with allowance for (13) and (16), it follows that

$$e^{2i(\varphi_+ - \varphi_-)} = e^{2i(\nu_- - \nu_+)}\frac{u + 2ikS}{u - 2ik(S+1)}. \tag{23}$$

From this equality, taking into account the definition (16) of $\varphi_\pm$, we get

$$\frac{\eta_+^2}{\eta_-^2} = \frac{u_1^2 + E(2S + 1 - 2n)^2}{u_1^2 + E(2S + 1 + 2n)^2} \tag{24}$$

Solving this equation together with (15), we get

$$\eta_\pm^2 = \frac{u_1^2 + E(2S + 1 \mp 2n)^2}{u_1^2 + E[(2S+1)^2 - 4n(1-n)]}. \tag{25}$$

In the determination of $\eta_\pm^2$ we used the equality of the moduli of the right and left sides of (23). The equality of the argument allows us to determine the function P(E) which enters into the expression for u. This is done literally in the same manner as in the Appendix of I. With thus, assuming that $k_F|a_\pm| \ll 1$, the corrections to the expression obtained there for P(E) turn out to be of the order of T^2, and in our case go beyond the limits of accuracy. We therefore assume, just as in I, that

$$P(E) = \frac{1}{b}(1 + a_+a_-E) - \frac{4k_F}{\pi}, \qquad b = \frac{a_+ - a_-}{2S + 1}. \tag{26}$$

We shall show below that a_+ and a_- determine the scattering amplitude at high temperatures, where it is not necessary to take into account the "Kondo effect" and therefore perturbation theory is valid. Accordingly, the $a_\pm$ are equal, apart from small correction terms, to the Born scattering amplitudes.

Summing all the results obtained above, we can finally represent the solution of the problem in the form

$$a_\pm = \frac{1}{2ik}[\eta_\pm e^{2i(\nu_\pm + \varphi_\pm')} - 1], \qquad \nu_\pm = \operatorname{arctg} ka_\pm,$$

$$\varphi_\pm' = -\frac{k}{4\pi}\int_0^\infty \frac{dE' \ln \eta_\pm^2(E')}{k'(E' - E)},$$

$$\eta_\pm^2 = \left\{\left[1 + a_+a_-E - \frac{4k_Fb}{\pi} - \frac{2bk^2}{\pi k_F}I(E)\right]^2 + Eb^2(2S + 1 \mp 2n)^2\right\}\left\{\left[1 + a_+a_-E - \frac{4k_Fb}{\pi} - \frac{2bk^2}{\pi k_F}I(E)\right]^2 + Eb^2[(2S+1)^2 - 4n(1-n)]\right\}^{-1},$$

$$I(E) = 2k_F\int_0^\infty dk'\frac{n(k'^2)}{k'^2 - E}. \tag{27}$$

Just as when T = 0, the obtained solution has no singularities for complex E lying on the physical sheet.

If we expand the solution in a series up to terms of second order in $a_\pm$, we get

$$a_\pm = a_\pm + ika_\pm^2 \mp \frac{2b^2}{\pi}\left(S + \frac{1}{2} \mp \frac{1}{2}\right)\int_0^\infty \frac{dE'n(E')k'}{(E' - E - i\delta)}. \tag{28}$$

With the aid of (28) we can easily obtain a formula for the amplitude F:

$$F = a + bS\sigma + ik(1 - 2n)[a^2 + b^2S(S+1) + (2ab - b^2)S\sigma]$$
$$+ \left[\frac{2b^2}{\pi}\int_0^\infty \frac{dE'n(E')k'}{E' - E} + 2b^2kni(1 - 2n)\right]S\sigma. \tag{29}$$

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the argumentation concerning the smallness of the phase volumes of the multiparticle state is incorrect. However, this is immaterial to us. First, actually we need the scattering amplitude only when $E \approx E_F$, and second, multiparticle intermediate states appear in scattering by impurities only near the Fermi surface, just as the "Kondo effect," they are, in particular, missing when $E_F = 0$.

Exactly the same expression for F is obtained also from (2) with the aid of perturbation theory.

The function I(E) which enters in (27) is investigated in detail in Appendix II. From formula (A.II.a) it follows that I reaches a maximum when $E = E_F$, equal to $\ln(8E_F\gamma/\pi T)$, where $\gamma = \exp C$ (C—Euler's constant). Therefore the quantities $\eta_\pm^2$ can be expanded in a series in $a_\pm$ and b, if the inequality

$$\frac{2|b|k_F}{\pi}\ln\frac{8E_F\gamma}{\pi T} \ll 1, \tag{30}$$

which is a criterion for the applicability of perturbation theory to our problem, is satisfied besides the condition $k|a_\pm| \ll 1$.

We are interested in the behavior of the amplitude at $E \approx E_F$. With this, exactly just as in I, the difference from the results of perturbation theory for the phases $\varphi_\pm'$ is the result of the integration region near the Fermi surface. Because of this, it is possible to greatly simplify the expressions for $\varphi_\pm'$ and $\eta_\pm^2$ and represent them in the form

$$\eta_\pm^2 = \left\{\left[1 - g\ln\frac{\sqrt{\zeta^2 + (\pi T)^2}}{E_F} - ga\left(\frac{\zeta}{T}\right)\right]^2 + \left(\frac{\pi g}{2}\right)^2(2S+1-2n)^2\right\}$$

$$\times\left\{\left[1 - g\ln\frac{\sqrt{\zeta^2 + (\pi T)^2}}{E_F} - ga\left(\frac{\zeta}{T}\right)\right]^2 + \left(\frac{\pi g}{2}\right)^2[(2S+1)^2 - 4n(1-n)]\right\}^{-1},$$

$$\varphi_\pm' = -\frac{1}{4\pi}\int_{-E_F}^{\infty}\frac{d\zeta'\ln\eta_\pm^2(\zeta')}{\zeta'-\zeta}, \tag{31}$$

where

$$\zeta = E - E_F, \quad g = \frac{2k_Fb}{\pi}\left[1 - \frac{4k_Fb}{\pi}(1-\ln 2)\right]^{-1};$$

$$a\left(\frac{\zeta}{T}\right) = \int_0^{\infty}dt e^{-t/2}\left(\frac{1}{t} - \frac{1}{1-e^{-t}}\right)\cos\frac{\zeta t}{2\pi T}. \tag{32}$$

In the derivation of (31) we used expression (A.II.8) for I(E). We shall now calculate the conductivity. The general expression for it can be written in the following manner (see, for example, the book by Ziman[9]):

$$\Sigma = -\frac{e^2\mathcal{N}}{n_0 k_F}\int dE\,\frac{E}{E_F}\frac{\partial n}{\partial E}\frac{1}{\sigma_{tr}}, \tag{33}$$

where $\mathcal{N}$ is the density of the conduction electrons, n_0 the density of the impurities, and σ_{tr} the "transport" collision cross section. In our case there is only s-scattering and therefore the cross section σ_{tr} coincides with the ordinary cross section, for which we can write the expression[6]

$$\sigma = 4\pi[|A|^2 + S(S+1)|B|^2] = \frac{4\pi}{k}\operatorname{Im}A, \tag{34}$$

where

$$\operatorname{Im}A = \frac{1}{2k(2S+1)}[(S+1)(1-\eta_+\cos 2\delta_+) + S(1-\eta_-\cos 2\delta_-)]. \tag{35}$$

We shall first calculate Σ at high temperatures, when the condition (30) is satisfied. In this case $\eta_\pm^2 \approx 1$,

$\varphi_\pm' \ll 1$, and using (27) we get

$$(\operatorname{Im}A)^{-1} \approx \frac{4\pi}{k_F\sigma_0}\left\{1 - \frac{\sigma_1}{\sigma_0}\frac{4bk_F}{\pi}\left[2 + \frac{1}{k_F}I(\zeta)\right]\right\}, \tag{36}$$

where $\sigma_0 = 4\pi(a^2 + b^2S(S+1))$ is the Born scattering cross section, and $\sigma_1 = 4\pi b^2S(S+1)$ is the spin-dependent part of this cross section. Substitution of this expression in (33) yields after straightforward but very cumbersome calculations the following result:

$$\Sigma = \Sigma_0\left[1 - \frac{4bk_F}{\pi}\frac{\sigma_1}{\sigma_0}\left(\ln\frac{\pi T}{2E_F\gamma} + 1\right)\right], \tag{37}$$

where $\Sigma_0 = e^2\mathcal{N}(n_0k_F\sigma_0)^{-1}$ is the conductivity calculated in first order perturbation theory. We note that expression (37) is written in a form such that it does not depend on the system of units chosen by us with $m = \frac{1}{2}$. The same will hold true also for all the subsequent formulas for the conductivity. Formula (37) makes more precise the result obtained by Kondo,[2] whose method does not make it possible to determine the numerical factor under the logarithmic sign.[7]

We now proceed to the region of low temperatures. In this region it is necessary to consider separately two cases: b > 0 and b < 0. The first case is simpler and we shall start with it.

For positive g (the sign of g coincides with the sign of b), the bracket containing the logarithm in expression (31) for $\eta_\pm^2$ is larger than unity for all ζ and T; these quantities can therefore be represented in the form

$$\eta_\pm^2 \approx 1 \mp 2\pi^2g^2\left(S + \frac{1}{2} \mp \frac{1}{2}\right)n(\zeta)\left(1 - g\ln\frac{\sqrt{\zeta^2 + (\pi T)^2}}{E_F}\right)^{-2}. \tag{38}$$

This expression is written with logarithmic accuracy; we have neglected in it the quantity $\alpha(\zeta/T)$, which is of the order of unity compared with the large logarithm.

With the aid of (38), the phases $\varphi_\pm'$ can be written as follows: $\varphi_+' = S\varphi_0$ and $\varphi_- = -(S+1)\varphi_0$, where

$$\varphi_0 = \frac{\pi g^2}{2}\int_{-E_F}^{\infty}\frac{d\zeta'n(\zeta')}{(\zeta'-\zeta)}\left(1 - g\ln\frac{\sqrt{\zeta'^2 + (\pi T)^2}}{E_F}\right)^{-2}. \tag{39}$$

By virtue of (33), $\varphi_0(\zeta)$ must be known when $\zeta \sim T$. We break up the integral that defines φ_0 into two parts: from $-E_F$ to $-CT$, and from $-CT$ to ∞, where $C \gg 1$ but $g\ln C \ll 1$. In the first region, the integrand can be written in the form $\zeta'^{-1}(1 - g\ln[\zeta']/E_F)^{-2}$. The corresponding integral can be usually calculated, and we get for φ_0 the expression

$$\varphi_0 = \frac{1}{2}\pi g^2\left\{\frac{1}{g}\frac{g\ln(CT/E_F)}{1-g\ln(CT/E_F)} + \int_{-CT}^{\infty}\frac{d\zeta'n(\zeta')}{(\zeta'-\zeta)}\left(1-g\ln\frac{\sqrt{\zeta'^2+(\pi T)^2}}{E_F}\right)^{-2}\right\}. \tag{40}$$

The second term of this expression can be neglected, as can be readily verified by recognizing that in order of magnitude it is equal to

$$\left(1 - g\ln\frac{T}{E_F}\right)^{-2}\left\{-\ln\left(C + \frac{\zeta}{T}\right) + C_1\right\},$$

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[6] The fact that the scattering cross section is determined by the amplitude F_R generally speaking calls for justification. That this is indeed the case it is easiest to verify by recalling that the conductivity can be expressed in the form of integrals of Green's functions, the expression for which contains F_R and F_A, but not F (from more details see [3]).

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[7] The parameter b is connected with the constant J, which determines the interaction in Kondo's paper [2], as follows: $b = mJ\Omega/2\pi$, where Ω is the value of the unit cell; with this $2bk_F/\pi = (3/2)J\mathfrak{N}_0/E_F$, where $\mathfrak{N}_0 = \mathfrak{N}\Omega$ is the number of conduction electrons per unit cell.

where $C_1 \sim 1$ and $\zeta \sim T$. In addition, in the approximation in question it is meaningless to take into account the quantity C under the logarithm sign. By virtue of these circumstances we can ultimately represent φ_0 in the form

$$\varphi_0 \approx \frac{1}{2} \pi g \frac{g \ln(T/E_F)}{1 - g \ln(T/E_F)}. \tag{41}$$

Substitution of (40) and (41) in (35), followed by substitution of the result in (33), leads to the following expression for the conductivity:

$$\Sigma = \Sigma_0 \left[1 + \frac{\sigma_1}{\sigma_0} \frac{gL(2 - gL)}{(1 - gL)^2} \right]^{-1}, \tag{42}$$

where $L = \ln(T/E_F)$. When $g|L| \ll 1$, expressions (42) and (37) coincide, with logarithmic accuracy. In addition, (42) is exactly equal to the expression for the conductivity following from [3]. This is caused by the fact that when $g > 0$ the results of the present paper, and also of I, coincide with logarithmic accuracy with the results of [3].

In the opposite limiting case $g|L| \gg 1$ we have $\Sigma = \Sigma_0 \sigma_0/(\sigma_0 - \sigma_1)$, that is, the conductivity is maximal and its value is the same as if there were no spin-dependent part of the interaction. This result coincides fully with the result obtained in I.

We now proceed to the case $b < 0$. In this case it is impossible to obtain an expression analogous to (42) and valid at all temperatures, since the quantity $1 - gL$ can vanish. We shall therefore consider separately two regions of temperature: high temperatures ($1 - gL \gg |g|$) and low temperatures ($gL - 1 \gg |g|$).

In the region of high temperatures the phases $\varphi'_\pm$ can be calculated accurately just as when $b > 0$, and the expressions for the phases coincide in both cases (only the constant C which enters into the intermediate manipulations should satisfy the conditions $C \gg 1$ and $gL(1 - gL)^{-1} \ln C \ll 1$. As a result, the conductivity is described as before by formula (42), which, however, is more convenient now to rewrite in the form

$$\Sigma = \Sigma_0 \frac{[a^2 + b^2 S(S + 1)]k_F^2}{a^2 k_F^2 + (\pi g/2)^2 S(S + 1)/(1 - gL)^2}. \tag{43}$$

The second term in the denominator of this expression should be small compared with unity and not with $a^2 k_F^2$, and therefore already in the region of applicability of (43) there are temperatures for which $\Sigma \ll \Sigma_0$, that is, the resistance increases strongly.

We now proceed to low temperatures ($(gL - 1) \gg |g|$). To calculate the phases $\varphi'_\pm$, we break up the integration region into two parts, just as when $b > 0$ (now the constant C should satisfy the conditions $C \gg 1$ and $g(gI - 1)^{-1} \ln C \ll 1$). As a result it turns out that the integrals from $-CT$ to ∞ are negligibly small, the integrals from $-E_F$ to $-CT$ can be readily calculated with logarithmic accuracy, and for the phases we have

$$\varphi_+' = -\frac{\pi}{2} - S b k_F + \frac{\pi g S}{2} \frac{1}{1 - gL},$$

$$\varphi_-' = \frac{\pi}{2} + (S + 1) b k_F - \frac{\pi g(S + 1)}{2} \frac{1}{1 - gL}. \tag{44}$$

With the aid of these expressions we obtain for the conductivity

$$\Sigma = \Sigma_0 \frac{\sigma_0}{\sigma_m} \left[1 + k_F^2 a^2 + \left(\frac{\pi g}{2}\right)^2 \frac{S(S + 1)}{(1 - gL)^2} \right], \tag{45}$$

where $\sigma_m = 4\pi/k_F^2$ is the maximum possible value of the cross section on the Fermi surface. We see that since $\sigma_0 \ll \sigma_m$, we get $\Sigma \ll \Sigma_0$ and the conductivity reaches a minimum at $T = 0$.

The obtained results are in qualitative agreement with the experimental data, according to which the resistance of the number of metals containing impurities with spin has, in the case of low impurity concentration, a maximum at $T = 0$ (see, for example, the book by Ziman[9]), but this maximum is by far not as sharp as follows from (45). This is apparently connected with the fact that the radius of the impurity i_0 is actually not small ($r_0 \sim k_F^{-1}$), and, in addition, there are no grounds whatever for assuming that the interaction of the electron with the impurity is small. Therefore the partial cross sections with the given values of the orbital angular momentum $l \sim 1$ should be of the order of k_F^{-2} even far from the Fermi surface, and consequently they cannot increase very strongly as $E \to E_F$.

In conclusion, the author is grateful to S. L. Ginzburg for a large number of interesting discussions.

APPENDIX I

In this Appendix we derive Suhl's unitarity condition (8). Using the standard technique, we obtain for the retarded scattering amplitude the following expression:

$$F_{R\alpha'\alpha}^{M'M}(E) = \frac{1}{4\pi} \sum_{n,m} e^{-(E_n - F)/T} \left(\frac{j_{\alpha'n'm} j_{\alpha mn}^+}{E_{mn} - E - i\delta} + \frac{j_{\alpha n'm}^+ j_{\alpha'mn}}{E_{nm} - E - i\delta} \right); \tag{A.I.1}$$

The indices n, n', and m denote here the states of the system, including the impurity spin projection; the states n and n' differ only in these projections, which are respectively M and M'.

From (A.I.1), in particular, it is easy to obtain an integral representation for F_I, analogous to the corresponding representation of I, from which follow the statements made in the main text concerning the analytic properties of the functions A and B. The wave functions of our system are of the form

$$\Psi_n(r_1 \ldots r_N) = \Phi_n(r_1 \ldots r_N) + \Psi_n^{(1)}(r_1 \ldots r_N), \tag{A.I.2}$$

where $\Phi_n(r_1 \ldots r_N)$ is the antisymmetrized product of plane waves corresponding to the fact that at infinity the influence of the center can be neglected, and $\Psi_n^{(1)}(r_1 \ldots r_N)$ is part of the wave function describing the scattering. Obviously, for large r_i the functions $\Psi_N^{(1)}$ decrease, which reflects the fact that far from the center its influence on the system is small. We note also that the wave functions (A.I.2) contain $V^{-N/2}$ as a common factor, where V is the volume of the system.

We now consider the matrix element

$$j_{nm} = (\Phi_n, j\Phi_m) + (\Phi_n, j\Psi_m^{(1)}) + (\Psi_n^{(1)}, j\Phi_m) + (\Psi_n^{(1)}, j\Psi_m^{(1)}). \tag{A.I.3}$$

Since j decreases the number of particles in system by unity, each of the terms in this formula can be represented in the form of an integral in all N coordinates of the electrons which are contained in the state n. With this, the integrand expression in the first term (A.I.3) has a part that remains finite for large r_i. The integral of this part makes the principal contribution, when $V \to \infty$, to the expression for the matrix element j_{nm}, inasmuch as in integration over all the r_i there

arises a factor V^N which cancels precisely the same factor in the denominator. At the same time, the integrands which correspond to the three remaining terms (A.I.3) decrease for large values of r_i and therefore there occurs no such cancellation of the volumes, and their contribution to j_{nm} can be neglected when $V \to \infty$. Thus we see that the matrix element j_{nm} can be calculated by using the wave functions of the unperturbed problem.

The foregoing considerations, of course, are valid only for states which pertain to the continuous spectrum of the system. At the end of this Appendix we shall discuss the question of bound states and we shall show that they are immaterial to us.

From (A.I.1) follows the inequality

$$i(F_R^+ - F_R)_{\alpha'\alpha}^{M'M} = \frac{1}{2}\sum_{nm} e^{\beta(F-E_n)}\{\delta(E_{mn}-E)j_{\alpha'n'm}j_{\alpha mn}^+$$

$$+ \delta(E_{nm}-E)j_{\alpha n'm}^+ j_{\alpha'mn}\}. \quad \text{(A.I.4)}$$

By virtue of the foregoing, the matrix elements of the operators j and j^+ can be calculated with the aid of the unperturbed wave functions. The energies E_n and E_m are obviously also the energies of the ordinary states of an ideal gas (it was shown in the main text of the article that in the calculation of F_R it is possible to carry out the Gibbs averaging with Hamiltonian H_0).

Let us consider the contribution made to (A.I.4) by the single-particle intermediate states. In this case in the first term the state m will differ from n in the presence of one additional particle with momentum k_1 and spin projection α_1; in addition, the spin projection of the impurity M_1 in the state m will also differ from the corresponding projections in the states n and n'. To the contrary, in the state m the particle (k_1, α_1) will not appear in the second term. We then get for the matrix element j_α,

$$j_{\alpha'n'm} = \langle n'|j_{\alpha'}a_{k_1\alpha_1}^+|n_1\rangle = \frac{1}{\sqrt{V}}\int dx e^{ikx}\langle n'|j_{\alpha'}\psi_{\alpha_1}^+(x)|n_1\rangle|_{x_0=-\infty}$$

$$= -\frac{1}{\sqrt{V}}\int d^4x \frac{\partial}{\partial x_0} e^{ikx}\vartheta(-x_0)\langle n'|\{\psi_{\alpha_1}^+(x), j_{\alpha'}(0)\}|n_1\rangle$$

$$= -\frac{i}{\sqrt{V}}\int d^4x e^{iEt}\left(i\frac{\partial}{\partial t} - H_0\right)\vartheta(t)\langle n'|\{j_{\alpha'}(t), \psi_{\alpha_1}^+(x,0)\}|n_1\rangle$$

$$= -\frac{4\pi}{\sqrt{V}}F_{R\alpha'\alpha_1}^{n,M'M_1}(E). \quad \text{(A.I.5)}$$

We have taken into account here the fact that there is no particle (k_1, α_1) in the state n', therefore $\langle n'|a_{k_1\alpha_1}^+ = 0$; in addition, we used the fact that the impurity is pointlike. The quantity $F_{R\alpha'\alpha_1}^{n,M'M_1}$ differs from the retarded scattering amplitude in that there is no Gibbs averaging in its definition F_R^n and F_R coincide when $T = 0$.

Using (A.I.5), and also the analogous expressions for the remaining matrix elements, we can write (A.I.4) in the form

$$i(F_R^+ - F_R)_{\alpha'\alpha}^{M'M} = \frac{2\pi^2}{V}\sum_{k_1\alpha_1 M_1 n} e^{\beta(F-E_n)}\{F_{R\alpha'\alpha_1}^{n,M'M_1}F_{R\alpha,\alpha}^{+nM_1M}(1-n_{k_1})$$

$$+ F_{R\alpha_1\alpha}^{+n,M'M_1}F_{R\alpha'\alpha_1}^{n,M_1M'}n_{k_1}\}\delta(k_1^2-E). \quad \text{(A.I.6)}$$

We have introduced here the additional factors n_{k_1} and $1-n_{k_1}$ ($n_{k_1} = 0$ and 1), which emphasize the

fact that in the first term in the initial state there is no particle with momentum k_1, and in the second term such a particle must be present in the initial state.

It now remains to carry out the Gibbs averaging in (A.I.6). We shall show now that the factors F_R^n and F_R^{+n} can be averaged independently. In fact, according to (A.I.5), F_R^n is expressed in terms of the diagonal matrix element of the operator $R = \{j_\alpha(t), \psi_{\alpha'}^+(x, 0)\}$. Obviously, this operator can be represented in the form

$$R = \sum_s V^{-s}\sum_{(p,q)} C_s(p_1 \ldots p_s; q_1 \ldots q_s)a_{p_1}^+ \ldots a_{p_s}^+ a_{q_1} \ldots a_{q_s}. \quad \text{(A.I.7)}$$

In the calculation of the diagonal matrix element R we must take into account only those terms in which there are pairs of operators $a_{p_1}^+$ and a_{p_1} pertaining to one state (p_1), since the terms containing, for example, the quartets of operators pertaining to one state make a contribution which vanishes as $V \to \infty$. In perfect analogy, when $V \to \infty$ there vanishes the contribution to the product $R_{nn}R_{nn}^+$ from those terms which contain pairs of identical operators, both in R_{nn} and R_{nn}^+, and this means that these operators can be independently averaged.

Further, after such an averaging the obtained values differ from F_R and F_R^+ only in the fact that they contain a definite number of particles with momentum k_1. However, the contribution of particles with any one momentum to F_R is of the order of N^{-1}, and therefore it can be neglected. The averaging with respect to k_1 is then carried in (A.I.6) in elementary fashion, and we obtain after integration with respect k_1:

$$i(F_R^+ - F_R)_{\alpha'\alpha}^{M'M} = 2k\{F_R F_R^+(1-n) + (F_R^{+T}F_R^T)^T n\}_{\alpha'\alpha}^{M'M}, \quad \text{(A.I.8)}$$

where only the spin indices of the electron, and not of the impurity, are transposed. Putting $F = A + BS \cdot \sigma$, we obtain from this formula directly (8).

A procedure analogous to the one just described can also be used to take into account the contribution made to the unitarity condition by multiparticle intermediate states. This gives rise to integration over the momenta of the particles in the intermediate states, and the phase volume corresponding to the region of integration is very small (for three-particle states it is proportional to the larger of the two quantities T^2 or $(E - E_F)^2$), and on this basis we neglect the contribution from the multiparticle states, just as when $T = 0$.

It is of interest to note that in the spinless case, when there are no multiparticle intermediate states, formula (A.I.8) is exact.

The corresponding expression for the amplitude F_R is of the form $F_R = a(1 - ika)^{-1}$, just as in the absence of the Fermi sphere. This can be verified also directly, by solving (6) by a method described in the author's paper [10].

The unitarity relation (A.I.8) includes the retarded amplitude for F_R, and not the "causal" F. This is essentially a reflection of the fact that the physical meaning is possessed by retarded quantities (for example, G_R), and "causal" quantities are auxiliary. It can be shown that the unitarity condition for F is of the form

$$i(F^+ - F) = 2k[F_R F_R^+(1-n) - (F_R^{+T}F_R^T)^T n]. \quad \text{(A.I.9)}$$

We shall stop to discuss briefly the question of the bound states. For simplicity we confine ourselves to

the case $T = 0$. Here, obviously, there can be bound states with $E < 0$ (E—energy of the single-particle state), but first, they make no contribution to the unitarity condition, and second, they lie far from E_F and are immaterial to us. There can be no bound states with $E \approx E_F$ (we are referring, of course, to genuine bound states, and not resonances). In fact, in all of space (with the exception of the point where the center is located) the wave functions of the system satisfy the free Schrödinger equation, and therefore when $E > 0$ they cannot describe finite motion of any of the particles. We note that this argumentation is valid in the case when there in one impurity in the system. If the impurities are distributed in the system with a finite density, then, generally speaking, a realignment of the Fermi surface is possible and formula (8) may turn out to be incorrect. However, a discussion of this question is beyond the scope of the present paper.

APPENDIX II

In this Appendix we calculate the function $I(E)$ which enters in (27) with $|\zeta|$, $T \ll E_F$ ($\zeta = E - E_F$). We perform the calculation with accuracy to terms of the order ζ inclusive, this being needed for the calculation of the thermal emf, which will be presented subsequently.

Let us consider the integral

$$\tilde{I}(E) = 2k_F \int_0^\infty \frac{dk' n(k'^2)}{k'^2 - k^2 - i\delta} = 2k_F T \int_0^\infty dk' \sum_\omega \frac{e^{i\omega\tau}}{(i\omega - k'^2 + E_F)(k'^2 - E - i\delta)}.$$
(A.II.1)

In the right side of this equality we have represented $n(k'^2)$ in the form of a sum over the frequencies (see [5]).

The integral $\tilde{I}(E)$ can be transformed as follows:

$$\tilde{I}(E) = 2k_F T \int_0^\infty dk' \sum_\omega \left\{ \frac{e^{i\omega\tau}}{(i\omega - \zeta)(k'^2 - E - i\delta)} + \frac{1}{(i\omega - k'^2 + E_F)(i\omega - \zeta)} \right\}$$

$$= i\pi \frac{k_F}{k} n(E) + 2k_F T \sum_\omega \int_0^\infty \frac{dk'}{(i\omega - k'^2 + E_F)(i\omega - \zeta)},$$
(A.II.2)

and since $I = \text{Re}\,\tilde{I}$, we have

$$I(\zeta) = 2k_F T \sum_\omega \int_0^\infty \frac{dk'}{(i\omega - k'^2 + E_F)(i\omega - \zeta)} = -i\pi k_F T \sum_\omega \frac{\varepsilon(\omega)}{(i\omega - \zeta)\sqrt{E_F + i\omega}}$$

$$= -\pi k_F T \sum_{\omega > 0} \frac{\omega}{\omega^2 + \zeta^2} \left(\frac{1}{\sqrt{E_F + i\omega}} + \frac{1}{\sqrt{E_F - i\omega}} \right)$$

$$- i\pi T k_F \zeta \sum_{\omega > 0} \frac{1}{\omega^2 + \zeta^2} \left(\frac{1}{\sqrt{E_F + i\omega}} - \frac{1}{\sqrt{E_F - i\omega}} \right),$$
(A.II.3)

where $I(\zeta)$ was broken up into two parts, one even in $\zeta (I_1)$ and one odd (I_2).

Let us consider first I_1. It can be written in the form

$$I_1(\zeta) = -\pi k_F T \sum_{\omega > 0} \frac{1}{\omega} \left(\frac{1}{\sqrt{E_F + i\omega}} + \frac{1}{\sqrt{E_F - i\omega}} \right)$$

$$+ \pi k_F T \sum_{\omega > 0} \frac{\zeta^2}{\omega(\omega^2 + \zeta^2)} \left(\frac{1}{\sqrt{E_F + i\omega}} + \frac{1}{\sqrt{E_F - i\omega}} \right).$$
(A.II.4)

In these sums $\omega = \pi T(2n + 1)$. When $|\zeta|$, $T \ll E_F$, we can make in the second term the substitution $\sqrt{E_F \pm i\omega} \approx k_F$; as a result we get for it

$$2\pi T \zeta^2 \sum_{\omega > 0} \frac{1}{\omega(\omega^2 + \zeta^2)} = x^2 \sum_{n=0}^\infty \frac{1}{(n + \frac{1}{2})[(n + \frac{1}{2})^2 + x^2]}$$

$$= \frac{1}{2} \sum_{n=0}^\infty \left(\frac{2}{n + \frac{1}{2}} - \frac{1}{n + \frac{1}{2} + ix} - \frac{1}{n + \frac{1}{2} - ix} \right)$$

$$= \frac{1}{2}[\psi(\frac{1}{2} + ix) + \psi(\frac{1}{2} - ix) - 2\psi(\frac{1}{2})],$$
(A.II.5)

where $x = \zeta(2\pi T)^{-1}$, and ψ is the logarithmic derivative of the Γ function (see the book of Gradshteĭn and Ryzhik[11]).

We now calculate the first term in (A.II.4). To this end, we break up the sum over ω into two parts, from $\omega = \pi T$ to $\omega = \pi T(N - \frac{1}{2})$, and from $\omega = \pi T(N + \frac{1}{2})$ to infinity, choosing N in such a way, that $1 \ll N \ll E_F(2\pi T)^{-1}$. In the first part we can replace $\sqrt{E_F \pm i\omega}$ by k_F, after which it is equal to $-\ln 4N\gamma$ (see [11]), where $\gamma = \exp C$ (C is Euler's constant). In the second part, the sum can be replaced by an integral, which can be readily evaluated and which is equal to $\ln(\pi TN/2E_F)$. Combining the two results and taking (A.II.5) into account, we obtain

$$I_1(\zeta) = \ln \frac{\pi T}{8E_F\gamma} + \frac{1}{2}\left[\psi\left(\frac{1}{2} + \frac{\zeta i}{2\pi T}\right) + \psi\left(\frac{1}{2} - \frac{\zeta i}{2\pi T}\right) - 2\psi\left(\frac{1}{2}\right) \right].$$
(A.II.6)

the odd part $I_2(\zeta)$ can be calculated in perfect analogy. It is of the form

$$I_2(\zeta) = -\frac{\zeta}{2E_F} I_1(\zeta) - \frac{\zeta}{2E_F}.$$
(A.II.7)

Using the definition of the functions ψ, we can represent the function $I_1(\zeta)$ in the following fashion:

$$I_1(\zeta) = \ln \frac{\sqrt{\zeta^2 + (\pi T)^2}}{4E_F} + \int_0^\infty dt e^{-t/2} \left(\frac{1}{t} - \frac{e^t}{e^t - 1} \right) \cos \frac{\zeta t}{2\pi T}$$
(A.II.8)

$$= \ln \frac{\pi T}{8E_F\gamma} + \int_0^\infty dt e^{-t/2} \frac{1}{1 - e^{-t}} \left(1 - \cos \frac{\zeta t}{2\pi T} \right).$$

These expressions were used in the main text of the article.

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Translated by J. G. Adashko
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